# Space Propulsion and Power

**8 March 2012**

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***Integrity ★ Service ★ Excellence***

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## BRIEF DESCRIPTION OF PORTFOLIO:

***Multi-disciplinary (Propulsion, Materials, Plasma and Electro-Energetic Physics, Chemistry, etc), multi-physics, multi-scale approach to complex space propulsion problems***

## SUB-AREAS IN PORTFOLIO:

- **Coupled Materials and Plasma Processes Far From Equilibrium**

  ***with Sayir, Harrison (RSA), and Luginsland (RSE)***

- **Novel Energetic Materials**

  ***Multi-agency Coordination Committee: Petris/DTRA, Doherty/DHS, Anthenien/ARO, Bedford/ONR, Spowart, Hawkins/AFRL, Palaszewski, Fletcher, Sayir/NASA, Pagoria/LLNL, Owrutsky/NRL, Birkan, Berman/AFOSR***

- **Nonlinear, multi-scale, multi-physics high pressure combustion dynamics**

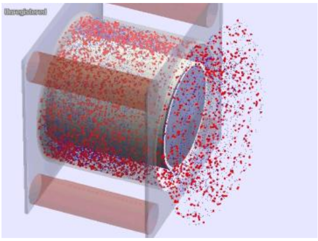
  ***with Fahroo (RSL), Darema (CC), and Li (RSA)***

# Coupled Materials and Plasma Processes Far From Equilibrium

Kick-off meeting, NASA Glenn RC, 29-30 November 2011

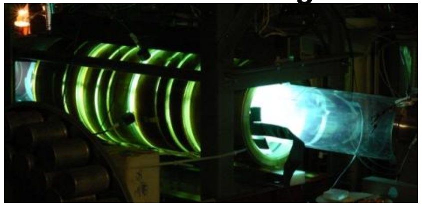
*with Sayir, Harrison (RSA), and Luginsland (RSE)*

**steady-state powered low-density plasmas**
**~ $10^{15}$ #/cm3**

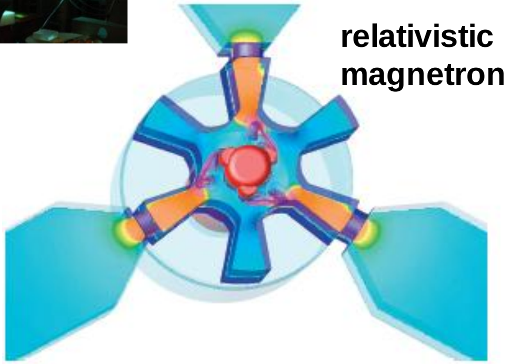


electric thrusters

Reverse field configuration



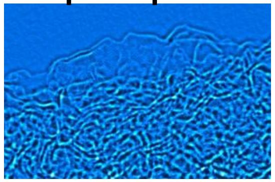
**Pulsed-powered relatively low-density plasmas, ~ $10^{13\text{-}20}$ #/cm3**



relativistic magnetron

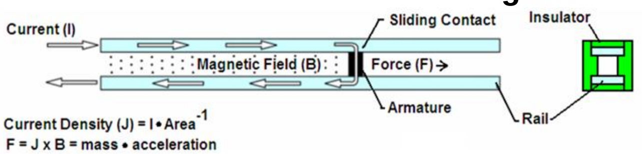
**Plasma/Electrode Interactions in High Current Density Environments (HPM sources)**
**500kV, 10kA, GW-class EM fields, 100ns to 1$\mu$s**

supercapacitor

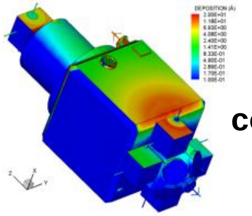


**Pulsed-powered high-density thermal plasmas**
**Pressure ~ 10's Mpa, Temperature ~ 1-10 eV, Pulse time ~ 1 us – 1 m**

railgun




**Characterize Surface / particle Interactions in Space Environment to mitigate contamination, charging, thermal control, undesired optical backgrounds**



Satellite contamination /charging

# Understand and Model the interactions among the low pressure plasma, material, and energy flow

**TEAM 1**
Nasr M. Ghoniem(UCLA)
Dan Goebel (JPL)
Igor D. Kaganovich (Princeton)
Yevgeny Raitses (Princeton)
Shahram Sharafat (UCLA)
Brian Williams (Ultramet)
Richard Wirz (UCLA)

What are the relationships between surface architecture and secondary electron emission, and the damage energy fluence limits?

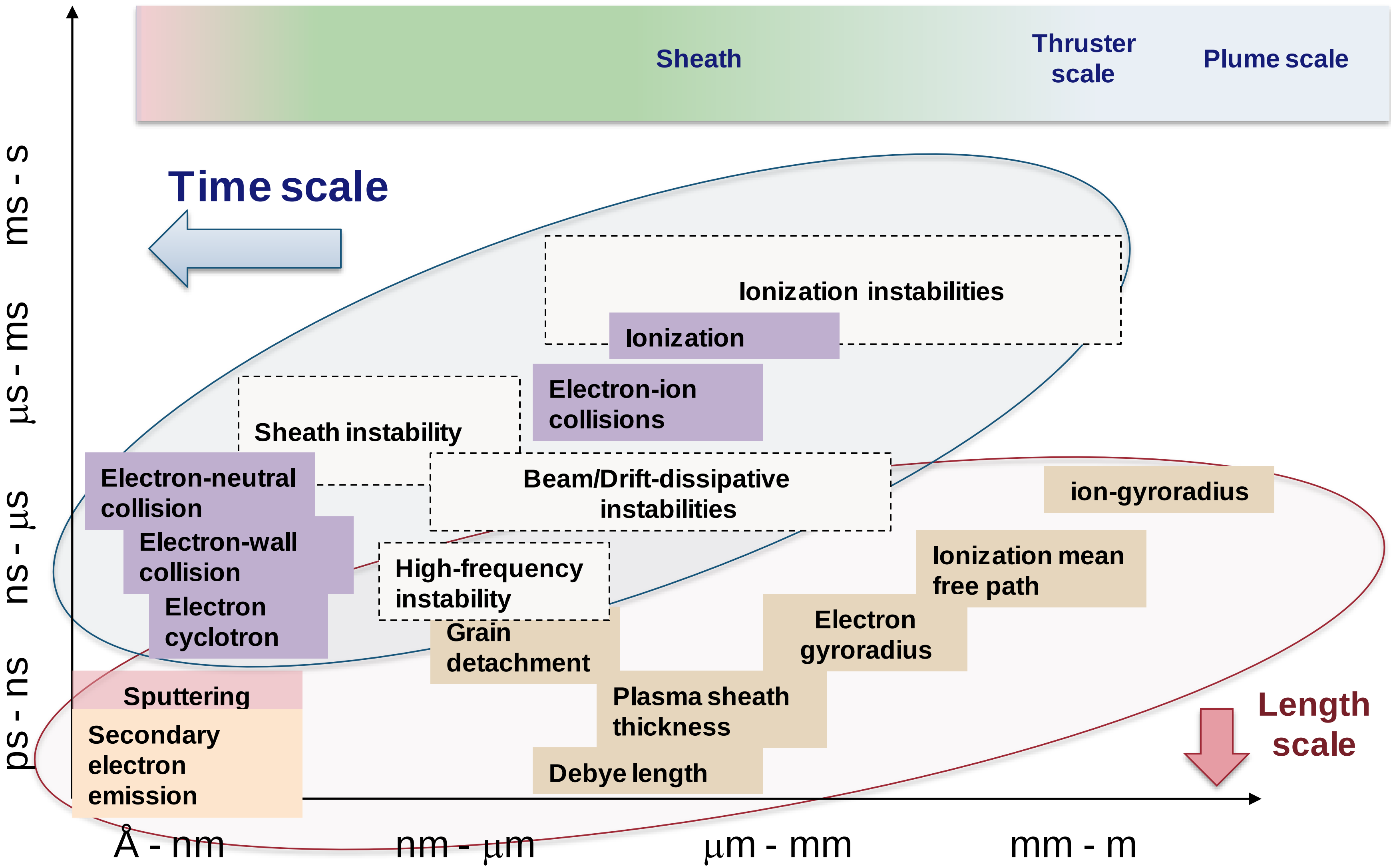
**TEAM 2**
Mitchell L. R. Walker (Georgia Institute of Technology)
Alex Kieckhafer (Georgia Institute of Technology)
Jud Ready (Georgia Tech Research Institute)
Greg Thompson (University of Alabama)

How to model plasma-material interaction to characterize grain detachment, sputtering leading to plasma modifications ?

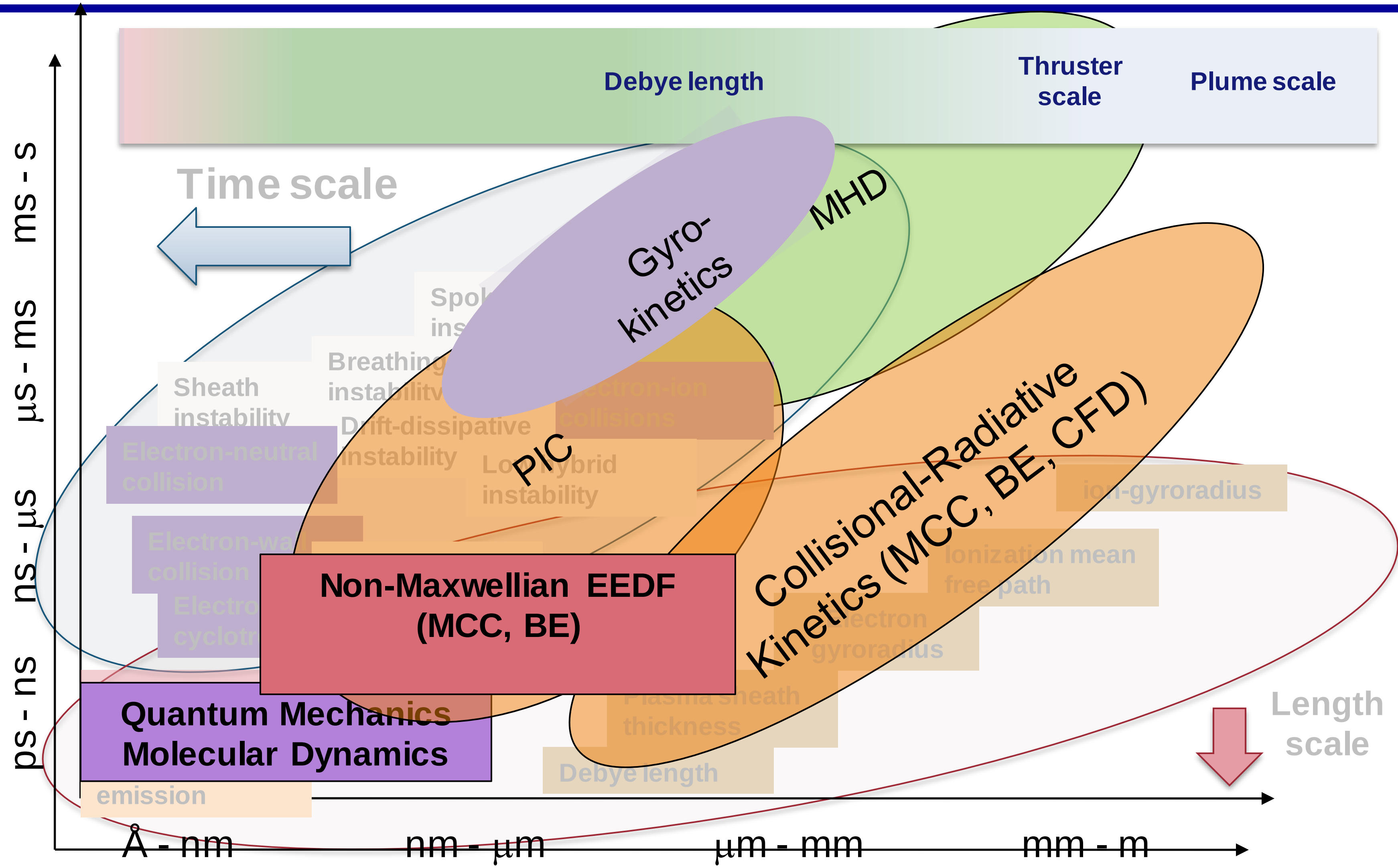
**TEAM 3**
Manuel Martinez-Sanchez (MIT)
Mark Cappelli (Stanford),
Dennis Whyte (MIT-PSFC)

What is the the effect of sheath instabilities, gas retention, and plasma-induced structural modifications on global performance ?

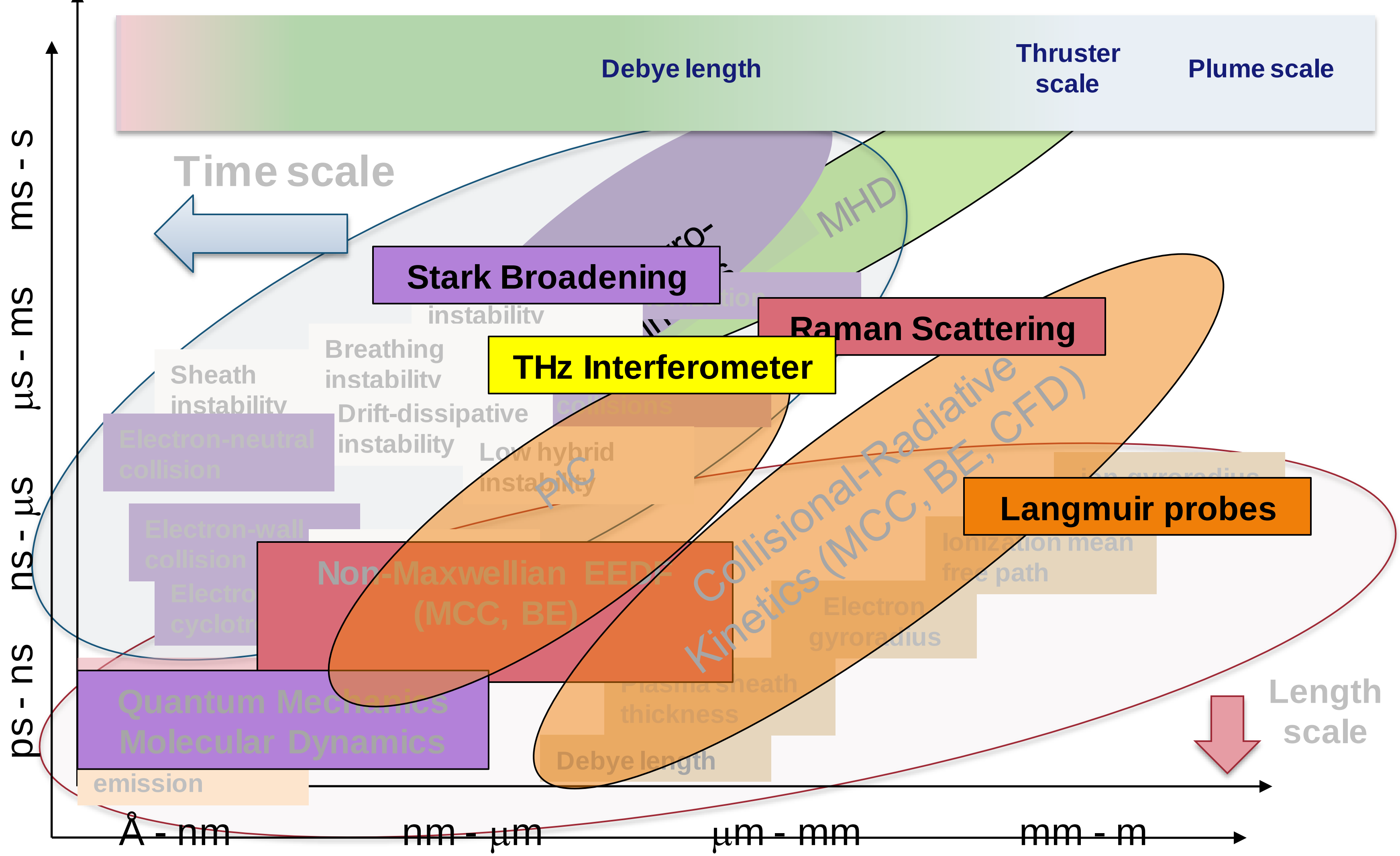
# Multiple Scales in low-density, steady-state powered plasmas



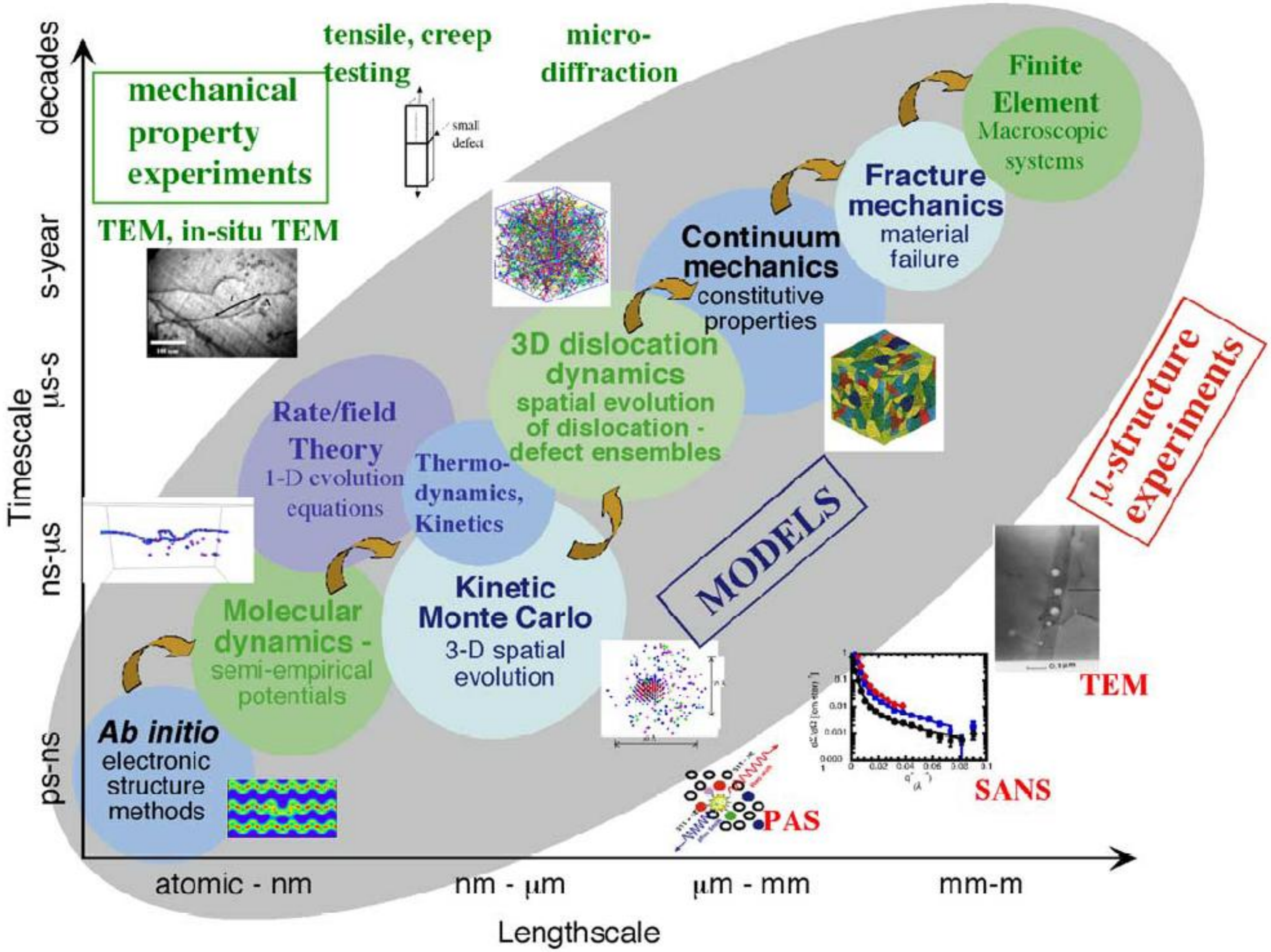
# Multiple Scales in low-density, steady-state powered plasmas - Computational Tools



# Multiple Scales in low-density, steady-state powered plasmas - Diagnostic Tools



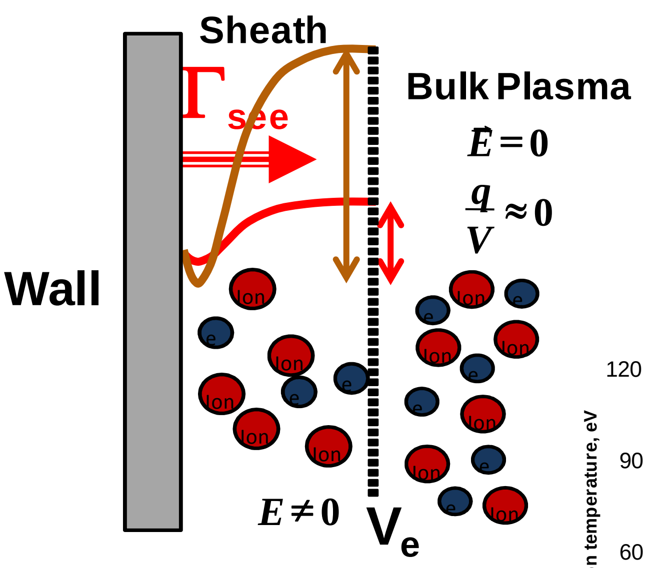
# Multi-scale Modeling of Materials



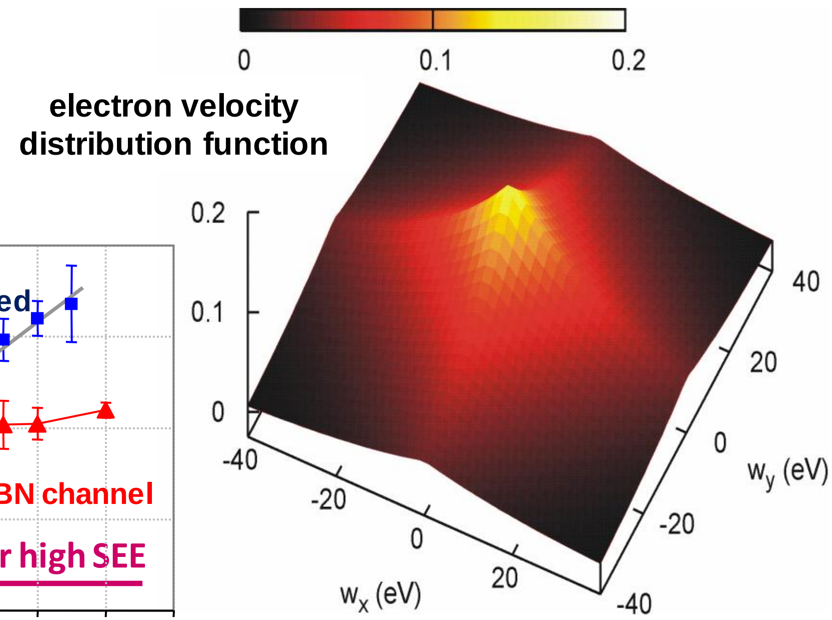

B. Wirth, 2004

# Example:
# Secondary Electron Emission: Good or Bad?

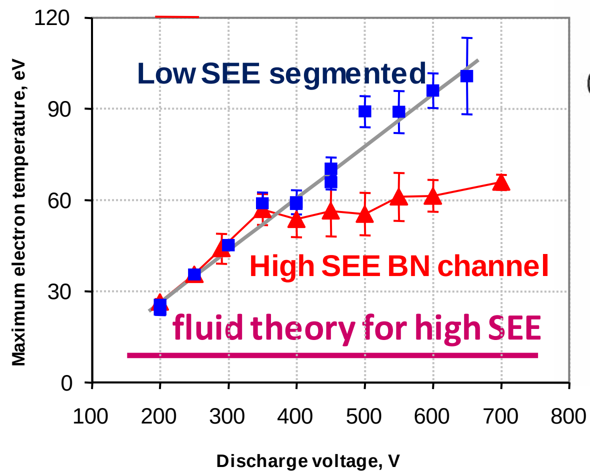
•***According to the Classic Fluid theory of Hobbs and Wesson, SEE is GOOD !!, leads to reduced wall erosion !!*** **Martinez – Sanchez / MIT (1997)**




•**Fluid theory assumes isotropic equilibrium (Maxwellian), and for walls with very high secondary electron emission, sheath collapses, sheat potential negligible !!**




**One Problem: can not predict the experimental results**




•***WHY?***

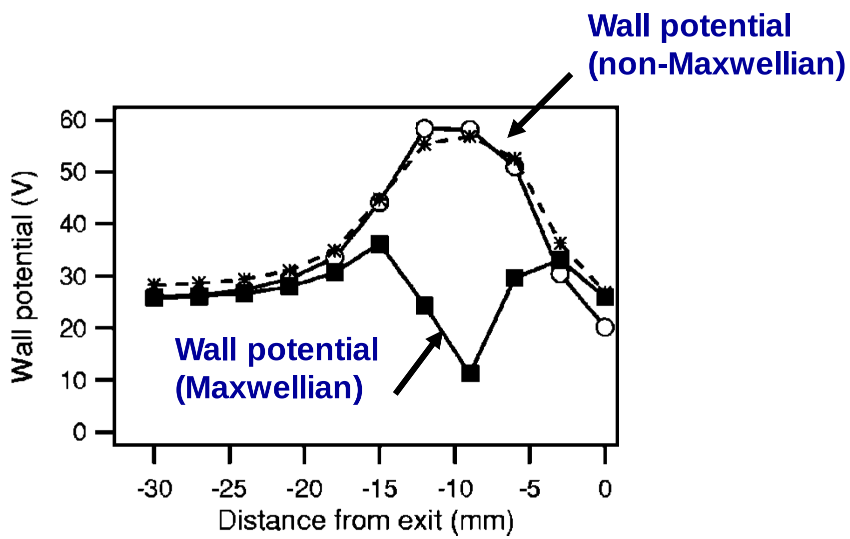
•**Plasma mean free path in thrusters are too high to achieve equilibrium (not enough electron-electron collisions)**

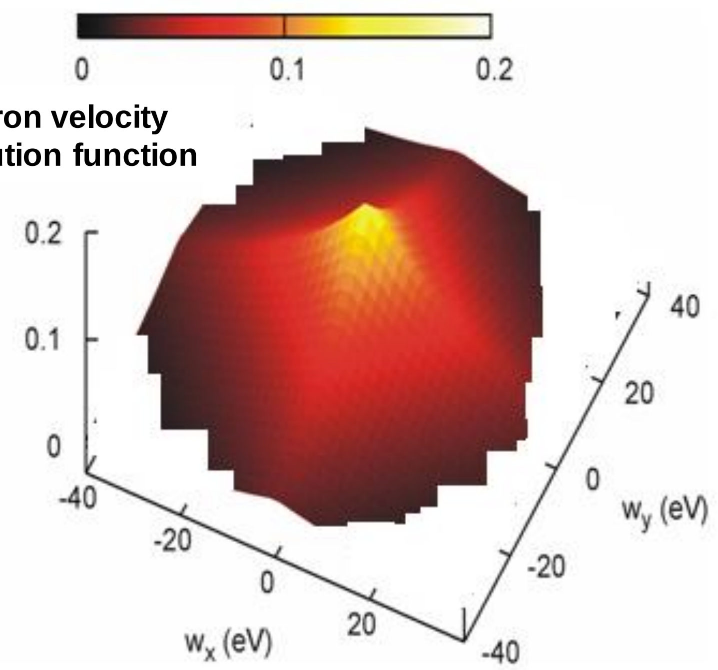
•**According to the fluid theory, maximum electron temperature does not change with discharge power due to huge electron heat flux to the wall**

# Model should account for Non-Equilibrium Effects !!

***Kinetic theory of Meezan and Cappelli / Stanford, High Secondary Electron Emission Depletes Tail of the Isotropic Electron Velocity Distribution***

- **Solution of the Boltzmann Equation, ISOTROPIC**



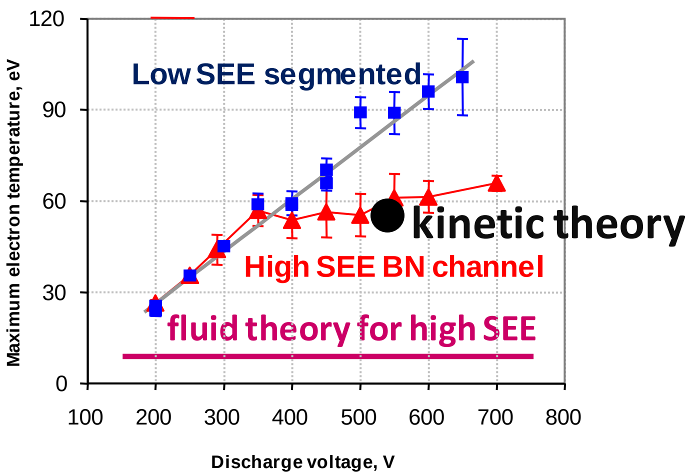

- **High Energy Electrons lost at wall**
- **Isotropic, can not predict secondary electron emission beams, and sheath instabilities**

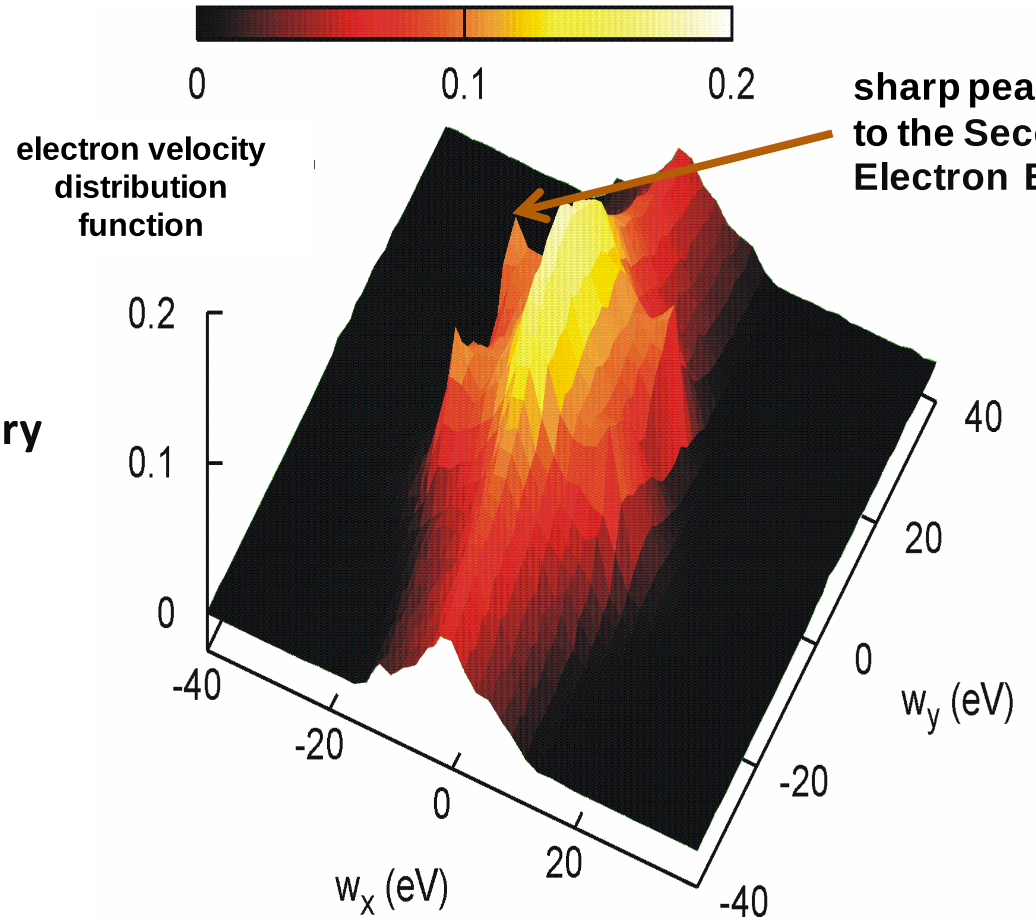
- **Sheath does not collapse, so Secondary Electron Emission has little effect on EROSION!**

## Example: Secondary Electron Emission: Good or Bad?

# Particle-In-Cell (PIC) simulations suggests that the electron velocity distribution function *is Anisotropic !!*

- Correctly predicts secondary electron emission beams, and sheath instabilities (Raitses, Kaganovich / Princeton)



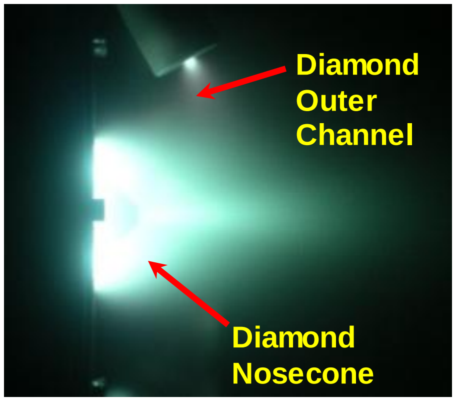




sharp peaks are due to the Secondary Electron Beams

- Secondary electron emission does not change the sheath potential
- Secondary electron beams cause instabilities near the sheath surface due to the "BUNCH UP"

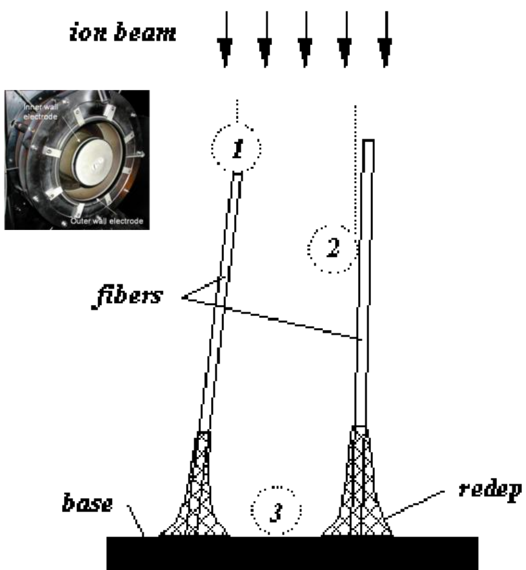
# Walls Made From Carbon-Based Materials with Different Micro and Macro Structures Can Have Very Different Effect On Plasma and Sheath Instabilities

**<u>Diamond Wall BHT-200 – Cappelli / Stanford (Secondary Electron Emission is unknown)</u>**




- Fundamental experiments verified high sputter resistance (GOOD!)
- Diamond (carbon) walls exaggerated plasma fluctuations – ***<u>plasma very UNSTABLE leading to VERY LOW THRUSTER EFFICIENCIES !!!</u>***

**<u>Carbon Velvet Wall– Raitses, Fisch, Kaganovich (Princeton) (has ZERO Secondary Electron Emission)</u>**




- Carbon velvet acts as almost ideal "black body" absorbing all incident particles preventing SEE
- With non-emitting carbon velvet walls, thruster operates more stable (no SEE induced instabilities of the plasma-sheath, attenuated breathing oscillations)
- With carbon velvet walls, the maximum electric field can be 2-3 times larger than with ceramic walls

- **Same element, different structure and architecture different result!**
- **<u>Hypothesis</u>: surface architecture affects performance!**

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- **Nonlinear, multi-scale, multi-physics high pressure combustion dynamics**

  *with Fahroo (RSL), Darema (CC), and Li (RSA)*

# Novel Energetic Materials

Workshop, 23-24 August 2011, Arlington, VA

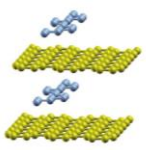
## The Sciences

Discovery, understand, model, and exploit novel energetics materials to obtain:

- Smart Responsive Materials
- Nanoenergetics
- Energetic Liquids, Oxidizers, and Binders

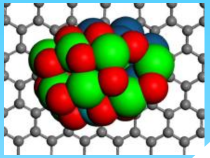
through Multiscale approach from the atomistic to macroscale

## Next Step

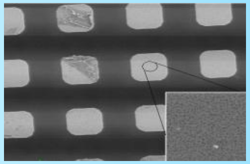


graphene sheets decorated with energetic organics and metallic nanoparticles for performance enhancement

encapsulated nanoscale fuels /catalysts, nanoporous fuel / oxidizer composites for control



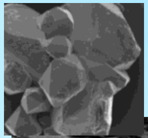
nPt
on graphene



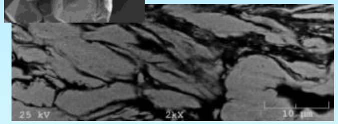
Ordered arrays of nano-porous silicone composites

surface functionalization , particle morphology, and defect reduction to decrease sensitivity

## Current S&T Effort

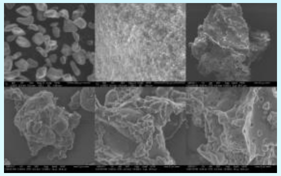


RDX with nano-Al encapsulated



Polystyrene coating Ammonium Borane

Frozen Propellants
Nickel Aluminum
Metal hydrides



## State-of-the-Art

Hydrogen and hydrocarbon, Ionic Propellants
ADN, HMX

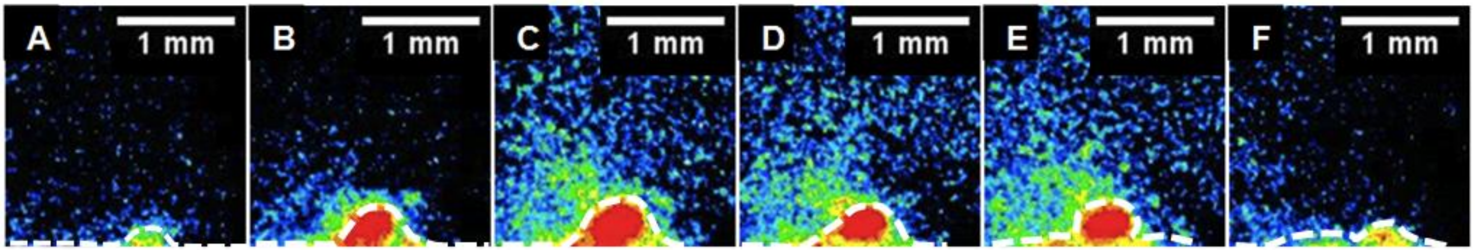
## Potential Impacts

- Mission tailored performance, and burning rate, switchable, smaller platforms
- Enhanced and new interactions with external stimuli for total control of reaction
- Reduced sensitivity, increased safety, and better mobility
- Enabled new missions

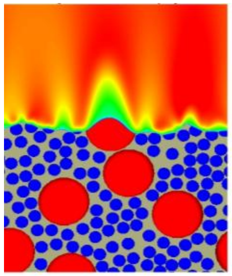
# High speed OH PLIF reveals that coarse ammonium perchlorate burns much faster at high pressures

•The diffusion flame structure changes from a jet-like to a lifted sheet-like diffusion flame as pressure is increased because of the relatively high local burning rate of the coarse AP

**1 atm:** Fluorescing coarse AP crystal is shown in red. Dashed line is the

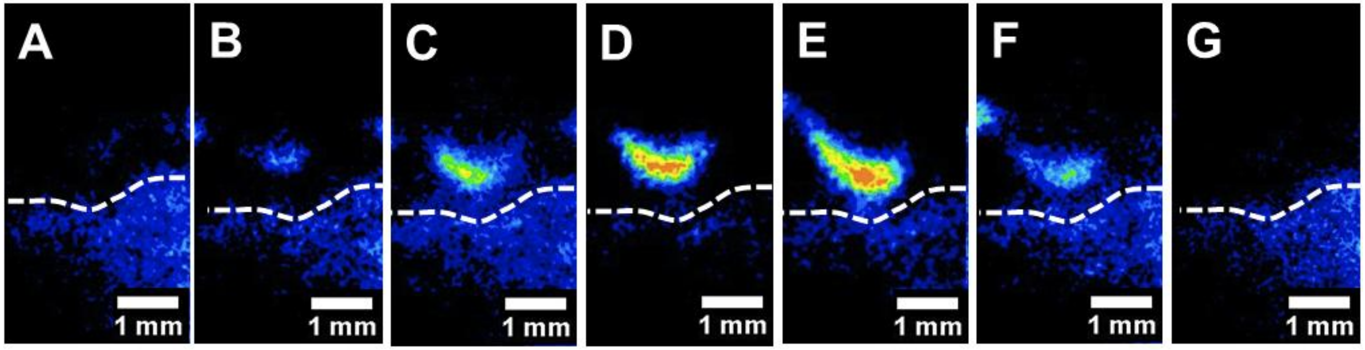



0 ms | 115.6 ms | 165.2 ms | 201 ms | 230 ms | 281 ms



State-of-the-Art 3-D simulation at high pressure (6 atm)

**6 Atm:** The relatively fast burning crystal cannot be seen because it is below the surface.



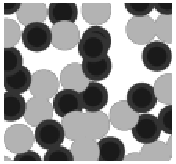

0.0 ms | 1.2 ms | 2.0 ms | 5.2 ms | 65.2 ms | 66.0 ms | 67.2 ms

•High speed OH PLIF also reveals that: Coarse AP is not affected by catalyst ($Fe_2O_3$ and CuO) addition, Catalyst should be inside coarse AP in order to have a greater affect on performance

# Nano-scale features affecting meso-scale behavior

# Example: mechanically activated Aluminum + Fluorocarbon mixture

**Al + polycarbon monofluoride Powder Mixture**



**Mechanical Activation**

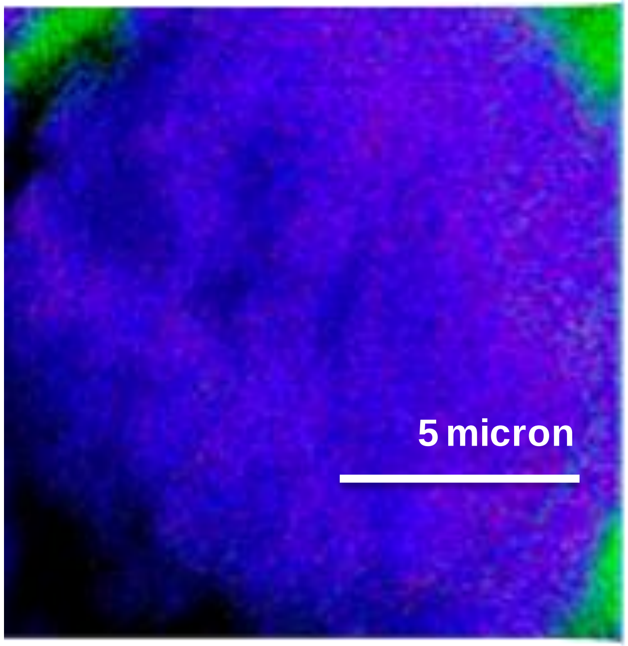
**Uniform composition and induced lattice defects (stored energy)**

SEM/EDX (Scanning Electron Microscopy/Energy DIspersive X-ray Spectroscopy)

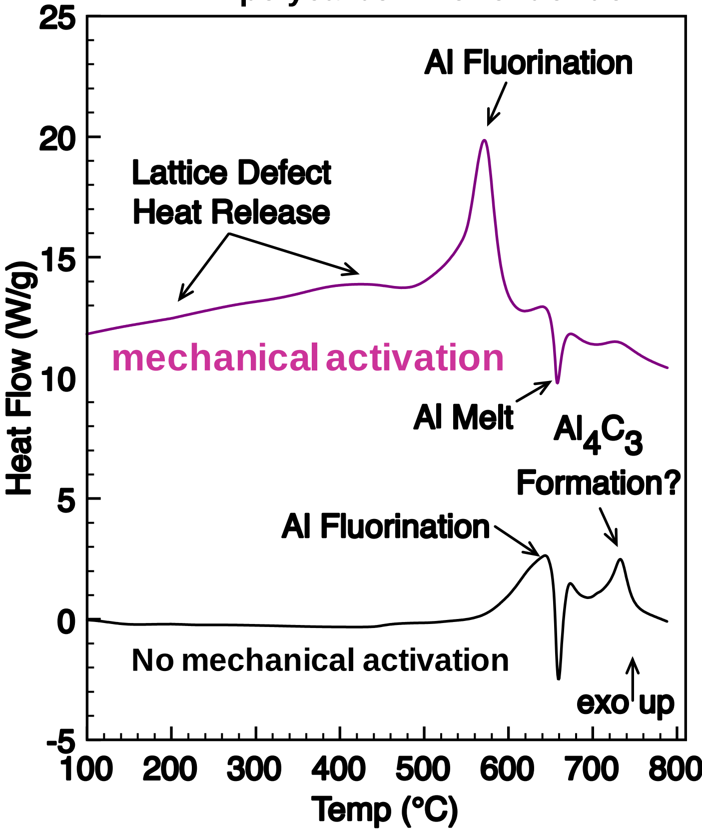
**Activated energetic particles**

**Aluminum=blue, Fluorine=red**

**Carbon=green**

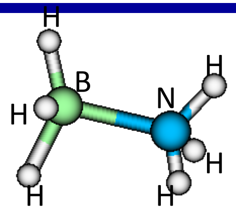



**DSC analysis of Al + polycarbon monofluoride**

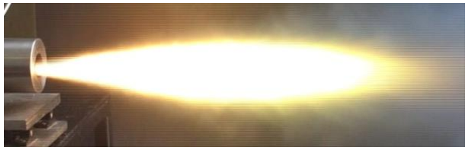



- **Fluorinated graphite encapsulated inside aluminum at nanoscales can provide increased combustion efficiency, reduced ignition temperature and agglomeration**

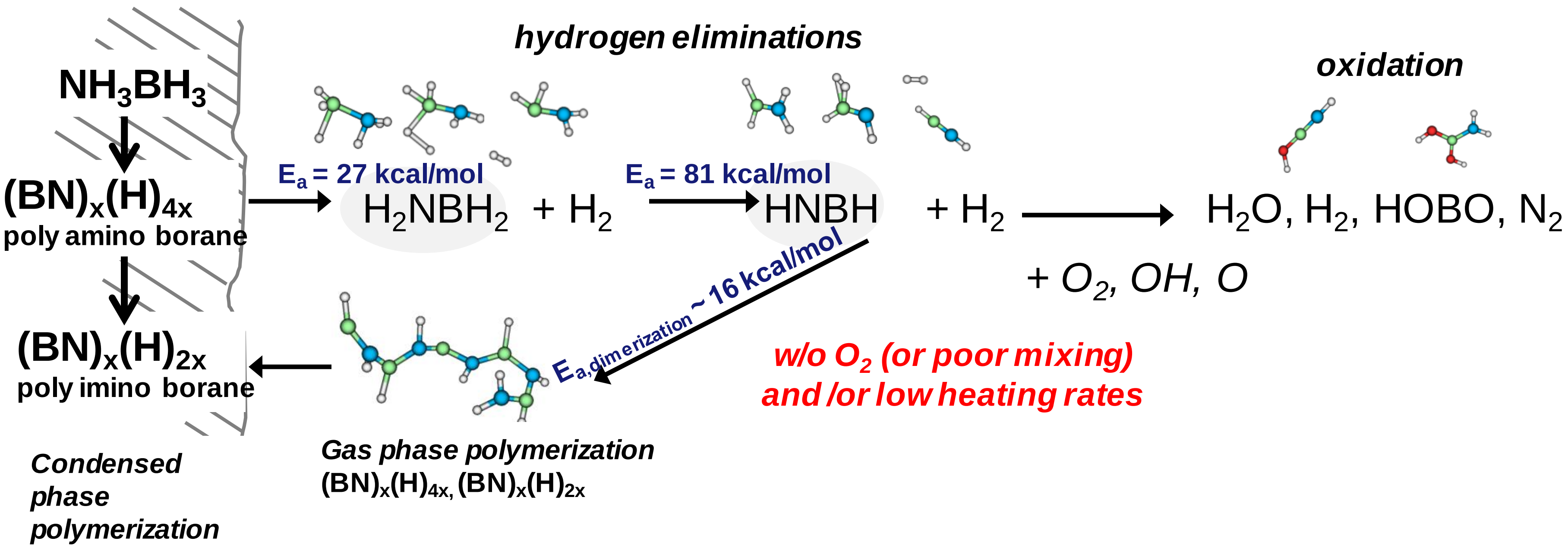
# Ammonia Borane ($NH_3BH_3$) as propellant additive, 20% hydrogen by mass, can significantly increase rocket performance




- **Ammonia Borane added to hybrid fuel (paraffin), $I_{sp,exp}$ increased ~10% with 20% mass addition**



- **<u>Problem</u>: Significant AB addition led to condensed phase product accumulation on fuel grain**
  - **<u>MD simulations, kinetic calculations, and TGA/DSC and Confined Rapid Thermolysis/FTIR/MS experiments</u>**




- **dehydrogenation of AB remains important in combustion processes at low temperature**
- **polymerization processes have lower energy barriers than dehydrogenation**
- **an ↑ in heating rate of 25x's results in a ↓of 2.6x's in mass accumulation in condensed-phase**
  - **<u>Hypothesis: Smaller ammonia borane particles may resolve the problem</u>**

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- **Nonlinear, multi-scale, multi-physics high pressure combustion dynamics**

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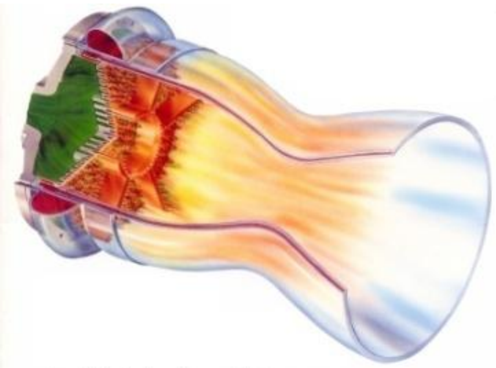
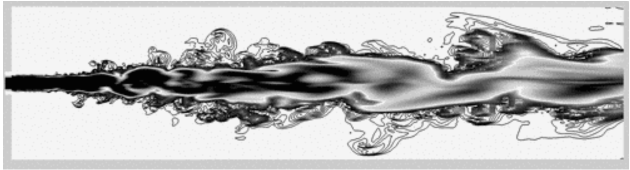
# Nonlinear, multi-scale, multi-physics high pressure combustion dynamics

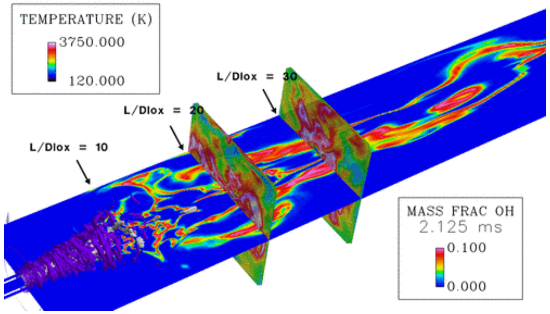
Workshop, 15 June 2011, London; Workshop, 23 August 2011, Arlington, VA

## PARADIGM SHIFT IN SIMULATION:



•Reduced Basis and Stochastic Modeling of a Complex High Pressure Combustion System to identify physical mechanisms responsible for the observed dynamical behavior

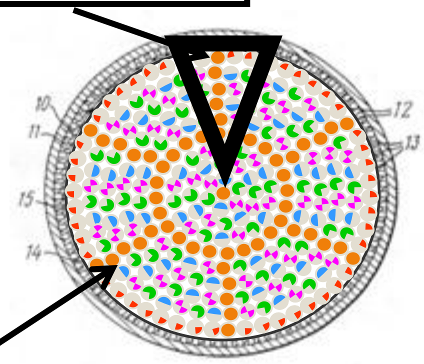


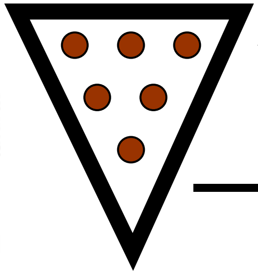



## PARADIGM SHIFT IN VALIDATION:

**Closed-loop actively controlled real-time hybrid approach**

Experimental domain



Boundary conditions=f(r,t)

Measured Pressure oscillation p'(t)

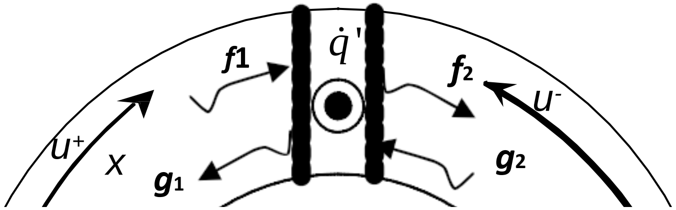
CONTROLLER

Computational domain="Remainder" of engine

# waves structure in a high pressure toroidal cavity with concentrated heat release zones

Zinn, Yang, Neumeier /Georgia Tech, and Law (Princeton)

•Consider a toroidal cavity with a single combustion point source. The acoustics is governed by the homogeneous wave equation except in the singular point.




•**Consider now the homogenous wave equation:**

$$\partial P'^2/\partial t^2 - \bar{C}^2 \partial P'^2/\partial x^2 = 0$$

$\lambda^R = x - ct$ **Right propagating characteristics** ➡ Right going pressure wave $p^R = f(\lambda^R)$ ➡ $u^R = \dfrac{f(\lambda^R)}{\bar{\rho}\bar{c}}$

$\lambda^L = x + ct$ **Left propagating characteristics** ➡ Left going pressure wave $p^L = g(\lambda^L)$ ➡ $u^L = \dfrac{g(\lambda^L)}{\bar{\rho}\bar{c}}$

•**With combustion:**

**The compact heat release source modifies the out going waves** ➡

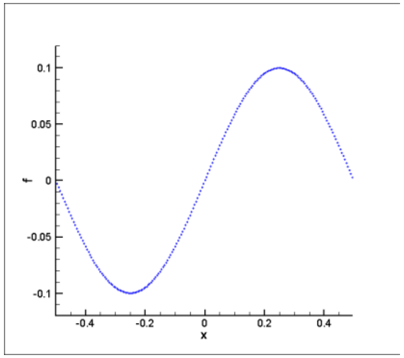
$$g_1 = g_2 + \frac{(\gamma - 1)}{2\bar{c} \cdot A} \cdot \dot{q}'$$

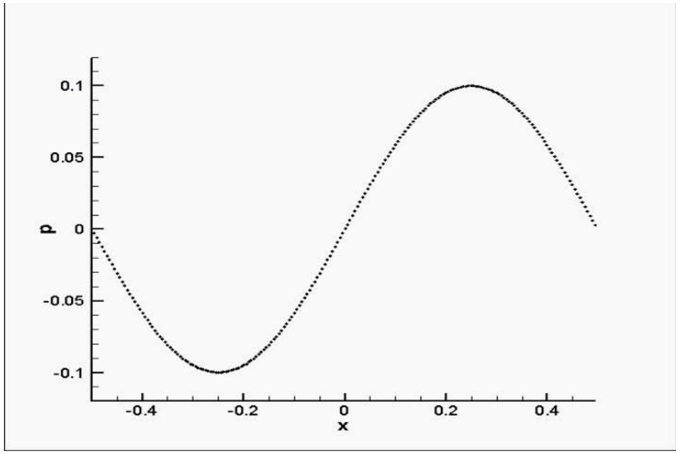
$$f_2 = f_1 + \frac{(\gamma - 1)}{2\bar{c} \cdot A} \cdot \dot{q}'$$

# The increased mean flow due to the convecting standing waves causes spinning waves with increasing amplitude leading to instability

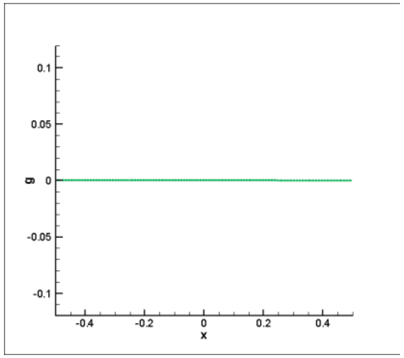
**If no tangential mean flow: spinning to a standing wave**

**Initial conditions**
**Right travelling wave f**



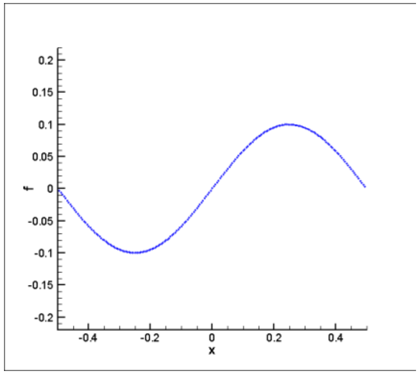



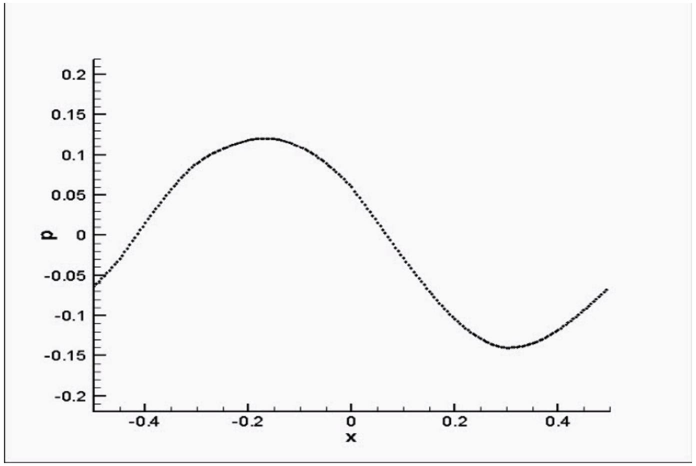

**Initial conditions**
**Left travelling wave g**



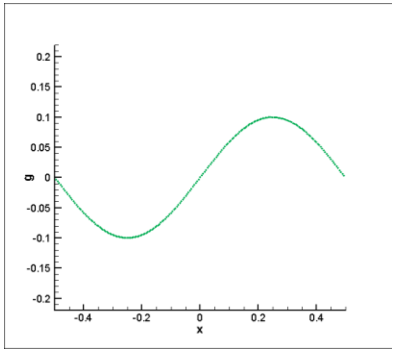

**TANGENTIAL MEAN FLOW due to recirculation near the injectors and inhomogeneous distribution of heat release, leading to convecting to a spinning wave**

**Initial conditions**
**Right travelling wave f**




**Initial conditions**
**Left travelling wave g**




- **Explained experimental results obtained at NASA (Marcus Heidmann , 1969)**

# Summary

***<u>Space Propulsion Portfolio has become a platform for Multi-disciplinary activities in all scales</u>:***

- Propulsion
- Materials
- Interface Sciences
- Plasma and Electro-Energetic Physics
- Applied and Computational Mathematics
- Chemistry
- and others…

***<u>Will provide the scientific foundation to:</u>***

- **Reduce Fuel Demand in Space / more efficient power generation and energy utilization, increase spacecraft lifetime, and reduce / control waste heat / provide novel design propellants / increase reliability and performance**
- **understand and manage High Energy Density**
- **Enable high-energy storage in ultra-capacitors with nanostructured components,**
- **and others…**